Access DB# 17570

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Peter Wong Examiner # : 6886 Date: 3/30/04
Art Unit: 1761 Phone Number 30 2-1411 Serial Number: 09/500,624
Mail Box and Bldg/Room Location: RTN 8A51 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

_____

Earliest Priority Filing Date: _____

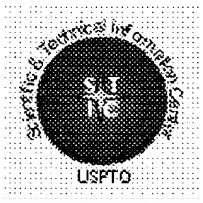
***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

****

STAFF USE ONLY	**Type of Search**		**Vendors and cost where applicable**	
Searcher: EL	NA Sequence (#)		STN	$237.32
Searcher Phone #:	AA Sequence (#)		Dialog	
Searcher Location:	Structure (#)	✓ (2) (subset)	Questel/Orbit	
Date Searcher Picked Up:	Bibliographic	✓ (and)	Dr.Link	
Date Completed: 4-1-04	Litigation		Lexis/Nexis	
Searcher Prep & Review Time: 5	Fulltext		Sequence Systems	
~~Clerical Prep Time:~~	Patent Family		WWW/Internet	
Online Time: 70	Other		Other (specify)	

PTO-1590 (8-01)

11/8/89



Request a Prior Art Search

Search requests relating to **published applications, patent families, and litigation** may be submitted by filling out this form and clicking on "Send."

For all other search requests, fill out the form, print, and submit the printout with any attachments to the STIC facility serving your Technology Center.

Tech Center:

○ TC 1600 ◉ TC 1700 ○ TC 2100 ○ TC 2600
○ TC 2800 ○ TC 3600 ○ TC 3700 ○ Other

Enter your Contact Information below:

Name: Leslie Wong
Employee Number: 68866 Phone: 571-272-1411
Art Unit or Office: 1761 Building & Room Number: Rem 8A51

Enter the case serial number (Required): 09/800624
If not related to a patent application, please enter NA here.

Class / Subclass(es) 426/535

Earliest Priority Filing Date: March 8, 2000

Format preferred for results:
☑ *Paper* ☐ *Diskette* ☐ *E-mail*

Provide detailed information on your search topic:

- In your own words, describe in detail the concepts or subjects you want us to search.
- Include synonyms, keywords, and acronyms. Define terms that have special meanings.
- *For Chemical Structure Searches Only*
  Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers
- *For Sequence Searches Only*
  Include all pertinent information (parent, child, divisional, or issued patent numbers) along with

h eb e c e ch b h

the appropriate serial number.
- *For Foreign Patent Family Searches Only*
  Include the country name and patent number.
- Provide examples or give us relevant citations, authors, etc., if known.
- FAX or send the **abstract, pertinent claims** (not all of the claims), **drawings, or chemical structures** to your EIC or branch library.

Enter your Search Topic Information below:

```
Compound of Formula I as attached in claim 1 as a flavor or
fragrance.  Specifically compounds of claims 2 and 3.

I already have the compound but it is not used as a flavor or
fragrance (GB 1409209).
```

Special Instructions and Other Comments:
(For fastest service, let us know the best times to contact you, in case the searcher needs further clarification on your search.)

Press ALT + F, then P to print this screen for your own information.

SEND RESET

h eb e c e ch b h

```
=> file reg
FILE 'REGISTRY' ENTERED AT 19:18:03 ON 01 APR 2004
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=> display history full l1-


     FILE 'LREGISTRY' ENTERED AT 18:55:09 ON 01 APR 2004
L1              STR

     FILE 'HCAPLUS' ENTERED AT 18:59:17 ON 01 APR 2004
L2            91 SEA GASSENMEIER ?/AU
L3           352 SEA GRAB ?/AU
L4            36 SEA GALOPIN ?/AU
L5           368 SEA BIGLER ?/AU
L6             0 SEA L2 AND L3 AND L4 AND L5
L7             3 SEA L2 AND L3
L8             0 SEA L2 AND L4
L9             0 SEA L2 AND L5
L10            0 SEA L3 AND L4
L11            0 SEA L3 AND L5
L12            0 SEA L4 AND L5
                 D L7 1-3 TI
                 SEL L7 1-3 RN

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L13          174 SEA (123-51-3/BI OR 124-13-0/BI OR 127-91-3/BI OR
L14           12 SEA L13 AND C H O S/ELF

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L15             STR

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L17          469 SEA SSS FUL L15
                 SAV L17 WON624/A
L18            7 SEA SUB=L17 SSS SAM L1
L19              STR L1
L20            0 SEA SUB=L17 SSS SAM L19
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     FILE 'CAOLD' ENTERED AT 19:11:44 ON 01 APR 2004
L22            1 SEA L21
L23           28 SEA L17
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L24           19 SEA L21
L25          356 SEA L17
L26       149834 SEA (FRAGRAN? OR PERFUM? OR PARFUM? OR COLOGNE? OR ODOR?
                 OR AROMA# OR SMELL? OR SCENT? OR OLFACT? OR REDOLENT? OR
                 ESSENCE? OR BOUQUET? OR AMBROS? OR ORGANOLEP?)/BI,AB
L27       206166 SEA (FLAVOR? OR FLAVOUR? OR SAVOR? OR SAVOUR? OR SAPID?
                 OR SAPOR? OR TAST? OR PALAT? OR GUSTAT? OR TOOTHSOME? OR
                 DELECTAB? OR SEASON? OR SPICE? OR APPETIZ? OR ORGANOLEP?)
                 /BI,AB
L28       917464 SEA (MIXT# OR MIXTURE? OR BLEND? OR ADMIX? OR COMMIX? OR
                 IMMIX? OR INTERMIX? OR COMPOSIT? OR COMPN# OR COMPSN# OR
                 FORMULAT? OR INTERSPER?)/TI

     FILE 'LCA' ENTERED AT 19:13:31 ON 01 APR 2004
L29        15216 SEA (MIX? OR BLEND? OR ADMIX? OR COMMIX? OR IMMIX? OR
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                 OR COMPOSIT? OR COMPN# OR COMPSN# OR FORMULAT? OR
                 COMBINAT? OR INTERSPER? OR AMALGAM?)/BI,AB

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L30        16571 SEA (L26 OR L27)(2A)L29
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L32            2 SEA L24 AND L27
L33            9 SEA L25 AND L26
L34            5 SEA L25 AND L27
L35            0 SEA (L31 OR L32) AND L28
L36            1 SEA (L31 OR L32) AND L30
L37            0 SEA (L33 OR L34) AND L28
L38            2 SEA (L33 OR L34) AND L30
L39            5 SEA L36 OR L31 OR L32
L40            6 SEA (L33 OR L34 OR L38) NOT L39

     FILE 'CAOLD' ENTERED AT 19:17:00 ON 01 APR 2004
L41           27 SEA L23 NOT L22

     FILE 'REGISTRY' ENTERED AT 19:18:03 ON 01 APR 2004


=> d l21 que stat
L15                STR
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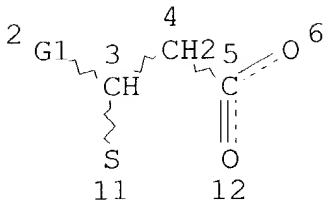

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
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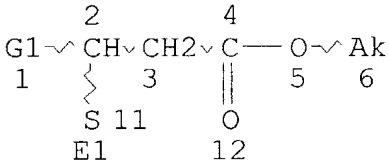
L19 STR



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CONNECT IS E1 RC AT 6
CONNECT IS E1 RC AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X8 C AT 6

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 273 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)


=> d l22 1 all hitstr

L22  ANSWER 1 OF 1  CAOLD  COPYRIGHT 2004 ACS on STN
AN   CA53:2092c  CAOLD
TI   quaternary ammonium compds.
AU   Ploetz, Ernst
PA   Badische Anilin- & Soda-Fabrik Akt.-Ges.
DT   Patent
     PATENT NO.    KIND         DATE
     ------------  -----------  ----
PI   DE 944130
IT  54051-19-3  98560-63-5
IT  54051-19-3  98560-63-5
RN   54051-19-3  CAOLD
CN   Butanoic acid, 3-mercapto-, methyl ester (9CI)  (CA INDEX NAME)
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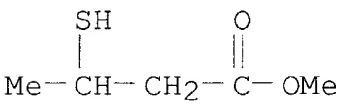

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RN   98560-63-5  CAOLD
CN   Butyric acid, 3-mercapto-, butyl ester (6CI)  (CA INDEX NAME)
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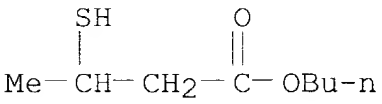

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=> d l41 1-27 ti

L41  ANSWER 1 OF 27  CAOLD  COPYRIGHT 2004 ACS on STN
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TI relations between the Cu atoms of ceruloplasmin - (I) studies on the exchange of 64Cu with ceruloplasmin, (II) interaction between the Cu binding sites

L41 ANSWER 2 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI synthesis of some potential antiradiation agents - (II) 1,3-thiazane derivs.

L41 ANSWER 3 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI thiochromone synthesis

L41 ANSWER 4 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI quaternary distilbazole compds.

L41 ANSWER 5 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI 7-sulfamidothiachroman 1,1-dioxides

L41 ANSWER 6 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI reaction of α-amino acids with acrylamide

L41 ANSWER 7 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI thiochromones with schistosomicide activity

L41 ANSWER 8 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI reaction of thiourea with α-bromobutyric acid - (II) peculiarities of the reaction at low concn. of starting materials

L41 ANSWER 9 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI ion-exchange chromatography of S amino acids and the sepn. of diastereoisomers

L41 ANSWER 10 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI thiophosphoric acid esters and pesticidal compns.

L41 ANSWER 11 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI quick-acting chem. balance

L41 ANSWER 12 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI addn. of mercaptoketones to reactive double bonds - (III) reactions with unsatd. carbonyl compds. and acid derivs.

L41 ANSWER 13 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI 3,3'-thioether dicarboxylic acids and their esters

L41 ANSWER 14 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI app. for the detn. in vacuo of the elec. cond. and Hall coeff. of thin metallic films and semiconductors
TI countercurrent distribution method for sepn. of chem. compds.

L41 ANSWER 15 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI photographic emulsions, antifogging agents for

L41 ANSWER 16 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI S-contg. amino acid

L41 ANSWER 17 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI antituberculous S compds. - (I) mercapto derivs. of alkanols, sulfides, and hydroxy sulfides

L41 ANSWER 18 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI Dieckmann reaction-prepn. of thiophenone derivs.

L41 ANSWER 19 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI phosphorothiolothionates from esters of alkene- and alkane-1,1-diols

L41 ANSWER 20 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI dithiophosphoric esters (heterocyclic)
TI heterocyclic dithiophosphoric esters

L41 ANSWER 21 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI synthesis of α- and β-(6-purinylthio)carboxylic acids

L41 ANSWER 22 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI β-thioethers of aliphatic aldehydes

L41 ANSWER 23 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI mineral acid salts of substituted isothiourea compds.

L41 ANSWER 24 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI antimetabolites - (I) synthesis and properties of sulfonic acid analogs of δ-aminolevulinic acid

L41 ANSWER 25 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI stabilization of poly(vinyl acetals)

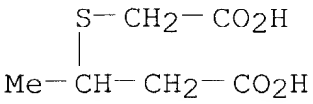
L41 ANSWER 26 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI flavor problem of soybean oil - (XIII) S coordination compds. effective in edible-oil stabilization

L41 ANSWER 27 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI thiazole series - (III) S-heterocyclic derivs. of 2-aminothiazole

=> d l41 26 all hitstr

L41 ANSWER 26 OF 27 CAOLD COPYRIGHT 2004 ACS on STN

AN CA51:7607g CAOLD
TI flavor problem of soybean oil - (XIII) S coordination compds. effective in edible-oil stabilization
AU Schwab, Arthur W.; Moser, H. A.; Gurley, R. S.; Evans, C. D.
IT 99-68-3 111-17-1 123-93-3 505-47-5 **4386-05-4**
5961-83-1 67242-91-5 92473-81-9 105910-65-4 119641-92-8
IT **4386-05-4**
RN 4386-05-4 CAOLD
CN Butanoic acid, 3-[(carboxymethyl)thio]- (9CI) (CA INDEX NAME)



=> file hcaplus
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=> d l39 1-5 ibib abs hitstr hitind

L39 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:798002 HCAPLUS
DOCUMENT NUMBER: 135:343645
TITLE: Preparation and use of ethyl 3-mercaptobutyrate as a **flavoring** or **fragrance** agent
INVENTOR(S): Dewis, Mark Lawrence; Edwards, David John; Kendrick, Lesley; Wright, Maria
PATENT ASSIGNEE(S): International Flavors + Fragrances Inc., USA
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001080666	A1	20011101	WO 2001-US12518	20010417

W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GE, HU, IN, IS, JP, KE, KG, KP, KR, KZ, LK, LR,

LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

GB 2363964	A1	20020116	GB 2000-9769	20000419
EP 1276390	A1	20030122	EP 2001-927136	20010417
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2002150662	A1	20021017	US 2001-7095	20011204
US 2004037787	A1	20040226	US 2003-645772	20030821

PRIORITY APPLN. INFO.:

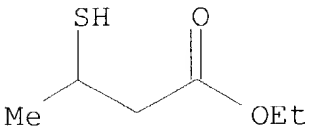
GB 2000-9769	A	20000419
WO 2001-US12518	W	20010417
US 2001-7095	B3	20011204

AB Et 3-mercaptobutyrate may be used in a wide variety of ingestible vehicles such as chewing gum compns., hard and soft confections, beverages, etc., to impart a green, mango, fruity **odor**. It may also be use in a **perfuming compn.** or a **perfumed** article as an active **perfuming** ingredient. Et 3-mercaptobutyrate is prepd. by reaction of Et crotonate with sodium hydrogen sulfide and sodium bicarbonate to form the disulfide dimer of Et 3-mercaptobutyrate followed by reducing the disulfide dimer to yield Et 3-mercaptobutyrate.

IT **156472-94-5P**
(prepn. and use of Et mercaptobutyrate as a **flavoring** or **fragrance** agent)

RN 156472-94-5 HCAPLUS

CN Butanoic acid, 3-mercapto-, ethyl ester (9CI) (CA INDEX NAME)



IC ICM A23L001-22

CC 17-6 (Food and Feed Chemistry)
Section cross-reference(s): 23, 62

ST mercaptobutyrate ethyl **flavoring fragrance**

IT Air fresheners
Beverages
Chewing gum
Colognes
Confectionery
Deodorants

Fabric softeners
Flavoring materials
Odor and **Odorous** substances
Perfumes
Shampoos
(Et mercaptobutyrate as a **flavoring** or **fragrance** agent)
IT Soaps
(Et mercaptobutyrate as a **flavoring** or **fragrance** agent)
IT Bath preparations
(gels; Et mercaptobutyrate as a **flavoring** or **fragrance** agent)
IT Detergents
(household cleaners; Et mercaptobutyrate as a **flavoring** or **fragrance** agent)
IT Detergents
(laundry; Et mercaptobutyrate as a **flavoring** or **fragrance** agent)
IT Mango (Mangifera indica)
(prepn. and use of Et mercaptobutyrate as a **flavoring** or **fragrance** agent)
IT **156472-94-5P**
(prepn. and use of Et mercaptobutyrate as a **flavoring** or **fragrance** agent)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

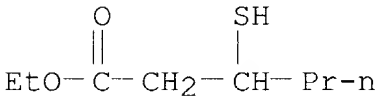
L39 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:742586 HCAPLUS
DOCUMENT NUMBER: 134:16811
TITLE: Quantitative Determination of Sulfur Containing Wine **Odorants** at Sub-ppb Levels. 1. Synthesis of the Deuterated Analogues
AUTHOR(S): Kotseridis, Yorgos; Ray, Jean-Loiec; Augier, Christian; Baumes, Raymond
CORPORATE SOURCE: Unite Biopolymeres Aromes, INRA-IPV, Montpellier, 34060, Fr.
SOURCE: Journal of Agricultural and Food Chemistry (2000), 48(12), 5819-5823
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB [2H10]-4-Sulfanyl-4-methylpentan-2-one (d10-SMP), [2H2]-3-sulfanylhexan-1-ol (d2-3SH), and [2H5]-3-sulfanylhexyl acetate (d5-3SHAc), the labeled analogs of impact **odorants**

of wines and other foods, were synthesized to be used for the quant. detn. of the natural compds. in white and red wines by stable isotope diln. assay. The sulfidation was achieved by Michael addn., on mesityl oxide or Et hex-2-enoate, resp., of the sulfhydryl anion generated in situ from triphenylsilanethiol and potassium fluoride under phase transfer conditions. The labeling of 4-sulfanyl-4-methylpentan-2-one (SMP) was obtained from the com. starting material, [2H6]acetone, so that this method could be used to synthesize 13C-labeled SMP from 13C-labeled acetone. The labeling of 3-sulfanylhexan-1-ol (3SH) and 3-sulfanylhexyl acetate (3SHAc) was obtained from redn. with lithium aluminum deuteride of the Michael adduct Et 3-sulfanylhexanoate and [2H3]-acetylation. During the synthesis, 3SH and 3SHAc were partially oxidized to their disulfide, which were reduced back to the thiols by an addnl. redn. step; the tertiary thiol SMP was less sensitive to this oxidn.

IT **309250-83-7**
(quant. detn. of sulfur contg. wine **odorants** at sub-ppb levels, synthesis of deuterated analogs)

RN 309250-83-7 HCAPLUS

CN Hexanoic acid, 3-mercapto-, ethyl ester (9CI) (CA INDEX NAME)



CC 17-11 (Food and Feed Chemistry)

ST sulfur compd wine **odorant** deuterated detn

IT Deuteration
Odor and **Odorous** substances
Wine analysis
(quant. detn. of sulfur contg. wine **odorants** at sub-ppb levels, synthesis of deuterated analogs)

IT 309250-80-4P 309250-81-5P 309250-82-6P
(quant. detn. of sulfur contg. wine **odorants** at sub-ppb levels, synthesis of deuterated analogs)

IT 7789-23-3, Potassium fluoride 17455-13-9, 18-Crown-6 ether
(quant. detn. of sulfur contg. wine **odorants** at sub-ppb levels, synthesis of deuterated analogs)

IT 128-37-0, 2,6-Di-tert-butyl-p-cresol, reactions 141-79-7, Mesityl oxide 1552-67-6, Ethyl hex-2-enoate 7704-34-9D, Sulfur, compds., reactions 14128-54-2, Lithium aluminum deuteride 14606-42-9, Triphenylsilanethiol 19872-52-7 51755-83-0 **309250-83-7**
(quant. detn. of sulfur contg. wine **odorants** at sub-ppb levels, synthesis of deuterated analogs)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE

IN THE RE FORMAT

L39 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:565917 HCAPLUS
DOCUMENT NUMBER: 103:165917
TITLE: Hair removal and waving with mercaptoisobutyric acid
INVENTOR(S): Pfleiderer, Ernst; Taeger, Tilman; Ude, Werner; Wick, Gertrud
PATENT ASSIGNEE(S): Rohm G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 27 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

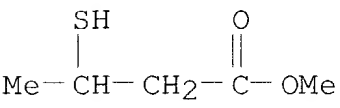
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3339104	A1	19850509	DE 1983-3339104	19831028

PRIORITY APPLN. INFO.: DE 1983-3339104 19831028

AB Cosmetic depilatories, hide dehairing prepns., and cold waving solns. contain β-mercaptoisobutyric acid [26473-47-2], its salts, and/or esters, and/or compds. that form these compds. in alk. medium. The hair prepns. contain 5-70 g active compd./100 mL liq. and have a pH of 6-13. A liq. depilatory contained Me β-mercaptoisobutyrate [**54051-19-3**] 100, CM-cellulose 3, propylene glycol 115, EtOH 42, **perfume** oil 10, and H2O 700 g.

IT **54051-19-3**
(cosmetic depilatories and waving prepns. and hide dehairing prepns. contg.)

RN 54051-19-3 HCAPLUS
CN Butanoic acid, 3-mercapto-, methyl ester (9CI) (CA INDEX NAME)



IC ICM A61K007-06
ICS A61K007-09; A61K007-155; C14C001-06
CC 62-3 (Essential Oils and Cosmetics)
Section cross-reference(s): 45
IT 26473-47-2 **54051-19-3**
(cosmetic depilatories and waving prepns. and hide dehairing prepns. contg.)

L39 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:427629 HCAPLUS
DOCUMENT NUMBER: 83:27629
TITLE: β-Mercaptoalkanoates for **perfumes** and **flavorants**
INVENTOR(S): Helmlinger, Daniel; Lamparsky, Dietmar; Schudel, Peter; Sigg-Gruetter, Trudi; Wild, Jost
PATENT ASSIGNEE(S): Givaudan, L., et Cie. S. A.
SOURCE: Patentschrift (Switz.), 4 pp. Division of Swiss 545,775 (See Ger. 2,155,672, CA 77: 100835j). CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

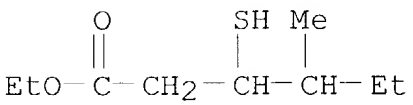
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 557423	A	19741231	CH 1973-3097	19701211

PRIORITY APPLN. INFO.: CH 1973-3097 19701211

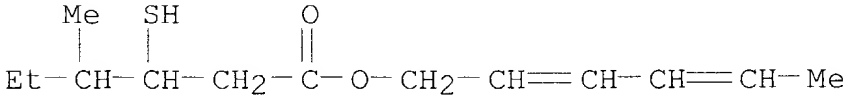
AB HSCHRCH2CO2R1 (I; R = pentyl, hexyl, heptyl, 1-heptenyl, EtCHMe, or Et2CH; R1 = Me, Et, cis-3-hexenyl, 2-hexenyl, or 2,4-hexadienyl), with fruity or flower-like **odors** were prepd. Thus, addn. of H2S to 50 g EtCMe:CHCO2Et gave, after purification, 47 g I (R = EtCHMe and R1 = Et), which had a light fruity **aroma.**

IT **37486-70-7P 37549-67-0P 37549-82-9P 37549-84-1P**
(prepn. of)

RN 37486-70-7 HCAPLUS
CN Hexanoic acid, 3-mercapto-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

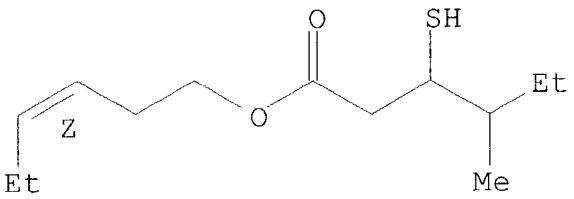


RN 37549-67-0 HCAPLUS
CN Hexanoic acid, 3-mercapto-4-methyl-, 2,4-hexadienyl ester (9CI) (CA INDEX NAME)

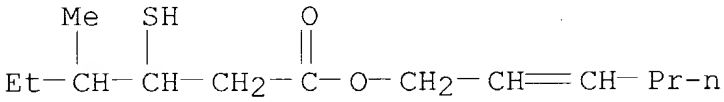


RN 37549-82-9 HCAPLUS
CN Hexanoic acid, 3-mercapto-4-methyl-, 3-hexenyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 37549-84-1 HCAPLUS
CN Hexanoic acid, 3-mercapto-4-methyl-, 2-hexenyl ester (9CI) (CA INDEX NAME)



IC C11B; A23L
CC 23-18 (Aliphatic Compounds)
Section cross-reference(s): 62
ST mercaptoalkanoate **perfume flavoring** agent;
alkanoate mercapto **perfume flavorant**
IT **Flavoring** materials
Perfumes
(mercaptoalkanoates for)
IT Esters, preparation
(of β-mercaptoalkanoic acids, with fruity or flower-like **aromas**)
IT 928-96-1P **37486-70-7P 37549-67-0P** 37549-75-0P
37549-76-1P 37549-77-2P 37549-78-3P 37549-79-4P 37549-81-8P
37549-82-9P 37549-83-0P **37549-84-1P**
(prepn. of)

L39 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:500835 HCAPLUS
DOCUMENT NUMBER: 77:100835
TITLE: Alkyl-and alkenyl 3-mercaptopropionates
INVENTOR(S): Helmlinger, Daniel; Lamparsky, Dietmar; Schudel, Peter; Sigg-Gruetter, Trudi; Wild, Jost
PATENT ASSIGNEE(S): Givaudan, L., et Cie. S. A.

SOURCE: Ger. Offen., 15 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

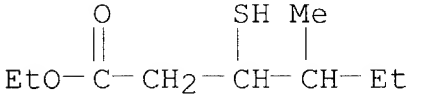
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2155672	A	19720629	DE 1971-2155672	19711109
DE 2155672	B2	19800508		
DE 2155672	C3	19810129		
CH 545775	A	19740215	CH 1970-18383	19701211
NL 7115451	A	19720613	NL 1971-15451	19711110
BE 776520	A1	19720612	BE 1971-111513	19711210
FR 2117625	A5	19720721	FR 1971-44385	19711210
GB 1336037	A	19731107	GB 1971-57456	19711210

PRIORITY APPLN. INFO.: CH 1970-18383 19701211

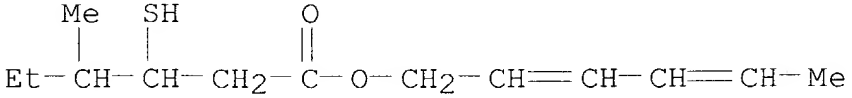
AB Nine R1CH(SH)CH2CO2R [I, R = Et, Me, (CH2)2CH:CHEt, CH:CHBu, CH2(CH:CH)2Me: R1 = C4-7 alkyl or CH:CH(CH2)4Me], us ed as **odorous** substances in **perfumes**, were prepd. by autoclaving R1CH:CHCO2R with H2S in alcs. in the presence of Na alkoxides or KOH or NaOH and hydroquinone or azobisisobutyronitrile. The compn. of a lavender-type **perfume** contg. I (R = Et, R1 = CHMeEt) was reported.

IT **37486-70-7P 37549-67-0P 37549-82-9P**
37549-84-1P
(prepn. of)

RN 37486-70-7 HCAPLUS
CN Hexanoic acid, 3-mercapto-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

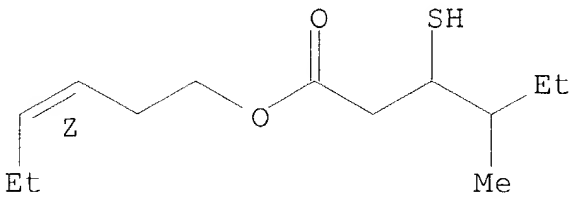


RN 37549-67-0 HCAPLUS
CN Hexanoic acid, 3-mercapto-4-methyl-, 2,4-hexadienyl ester (9CI) (CA INDEX NAME)

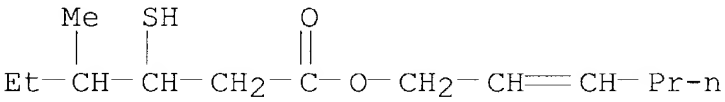


RN 37549-82-9 HCAPLUS
CN Hexanoic acid, 3-mercapto-4-methyl-, 3-hexenyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 37549-84-1 HCAPLUS
CN Hexanoic acid, 3-mercapto-4-methyl-, 2-hexenyl ester (9CI) (CA INDEX NAME)



IC C07C; C11B; A23L
CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 62
ST **perfume** mercapto ester aliph; hydrogen sulfide addn olefinic ester
IT **Perfumes**
(mercapto aliphatic esters for)
IT **37486-70-7P** 37549-66-9P **37549-67-0P**
37549-75-0P 37549-76-1P 37549-77-2P 37549-78-3P 37549-79-4P
37549-80-7P 37549-81-8P **37549-82-9P** 37549-83-0P
37549-84-1P 37645-98-0P
(prepn. of)

=> d l40 1-6 cbib abs hitstr hitind

L40 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
2002:808766 Document No. 138:170279 Synthetic equivalents of benzenethiol and benzyl mercaptan having faint **smell**: **odor** reducing effect of trialkylsilyl group. Nishide, Kiyoharu; Miyamoto, Tetsuo; Kumar, Kamal; Ohsugi, Shin-ichi; Node, Manabu (Kyoto Pharmaceutical University, Misasagi, Yamashina, Kyoto, 607-8414, Japan). Tetrahedron Letters, 43(47), 8569-8573 (English) 2002. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT

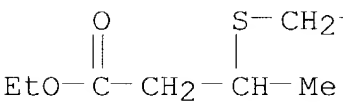
138:170279. Publisher: Elsevier Science Ltd..

AB Syntheses and **odor** tests of the 4-RC6H4X, 3-RC6H4X and 2-C6H4X (R = Me3Si, Et3Si, Pr3Si; X = SH, CH2SH) have revealed that the trimethylsilyl substituent on the benzene ring has a remarkable effect in reducing the foul **smell** of the parent benzyl mercaptan and benzenethiol. Protodesilylation allowed these silylated thiols to function as **odorless** synthetic equiv. of benzyl mercaptan and benzenethiol. The 4-Me3Si-substituted benzenethiol and benzyl mercaptan were tested as nucleophiles in Michael addn. reactions with R1HC:CR3COR4 (R4 = OEt; R1, R3 = H or Me; R4 = Et, R1 = Me, R3 = H) followed by protodesilylation to give corresponding phenylthio and phenylthiomethyl derivs. Radical addn. to PhC.tplbond.CCO2Et and 2-nitropropionate redn. reactions were also tested. Nucleophilic substitution of Br in 1-bromo-3-phenylpropane by 4-Me3SiC6H4SH was followed by halodesilylation, affording 4-iodo- and 4-bromo- derivs. This discovery will greatly improve the phys. environment of the researcher working with these malodorous compds.

IT **89529-96-4P 111731-00-1P**
(Michael addn. product; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

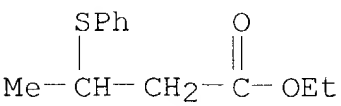
RN 89529-96-4 HCAPLUS

CN Butanoic acid, 3-[(phenylmethyl)thio]-, ethyl ester (9CI) (CA INDEX NAME)



RN 111731-00-1 HCAPLUS

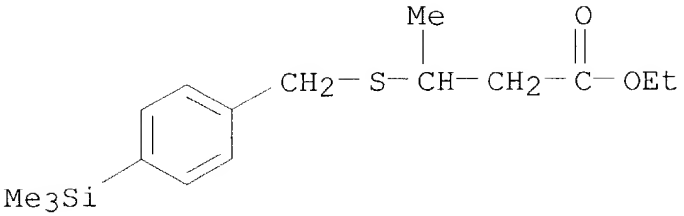
CN Butanoic acid, 3-(phenylthio)-, ethyl ester (9CI) (CA INDEX NAME)



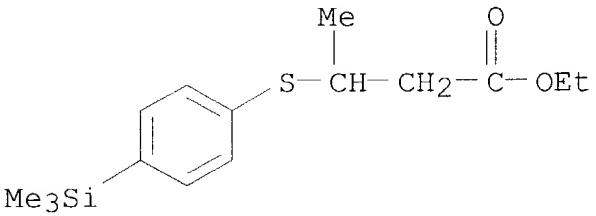
IT **497181-03-0P 497181-04-1P**
(protodesilylation; nucleophilic Michael addn. of silylated synthetic equiv. of benzyl mercaptans and thiophenols with subsequent protodesilylation)

RN 497181-03-0 HCAPLUS

CN Butanoic acid, 3-[[[4-(trimethylsilyl)phenyl]methyl]thio]-, ethyl ester (9CI) (CA INDEX NAME)



RN 497181-04-1 HCAPLUS
CN Butanoic acid, 3-[[4-(trimethylsilyl)phenyl]thio]-, ethyl ester (9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 21
ST benzenethiol benzylmercaptan synthetic equiv silyl deriv low **odor** prepn; silane deriv thiophenol benzenemethanethiol desilylation protonolysis bromination iodination; Michael condensation propiolate addn nucleophilic substitution silyl modified thiol; nucleophilic reaction silyl modified thiol low **odor** desilylation; thiol synthetic equiv nucleophilic reaction low **odor** product deprotection; green chem thiol mercaptan synthetic equiv low **odor**
IT Hydrolysis
(acid, protodesilylation; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)
IT Bromination
(bromodesilylation; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)
IT Substituent effects
(effect of trialkylsilyl substituent on **odor** of benzenethiols and benzyl mercaptans)
IT Iodination
(iododesilylation; prepn. of low-**odor** silylated

synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT **Odor** and **Odorous** substances
(nucleophilic Michael addn. of silylated synthetic equiv. of benzyl mercaptans and thiophenols with subsequent protodesilylation)

IT Thiols (organic), preparation
(**odor** scale, Michael addn., redn., nucleophilic substitution; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT Green chemistry
Michael reaction
Silylation
Substitution reaction, nucleophilic
(prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT Addition reaction
(radical; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their addn. and redn. reactions and desilylation)

IT Silylation
(retro; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 60805-64-3P **89529-96-4P 111731-00-1P**
241480-19-3P 377092-98-3P 497181-08-5P 497181-09-6P
497181-10-9P
(Michael addn. product; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 57337-85-6P
(Michael addn., **odor** scale; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 497180-93-5P 497180-94-6P 497180-95-7P
(Newman-Kwart rearrangement, thiolation; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 995-25-5
(arylation; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 13132-25-7 15288-53-6 17881-95-7
(carbamothioic acid esterification; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 30134-12-4P 497181-12-1P 497181-13-2P 497181-14-3P
(desilylation; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their substitution reactions and desilylation)

IT 17882-12-1P
(**odor** scale, Michael addn., radical addn., redn., desilylation; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 17881-83-3P 33356-45-5P 497180-78-6P 497180-79-7P
497180-80-0P 497180-81-1P 497180-82-2P 497180-83-3P
497180-84-4P 497180-85-5P
(**odor** scale; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 95-56-7, 2-Bromophenol 106-41-2, 4-Bromophenol 591-20-8, 3-Bromophenol 994-30-9, Chlorotriethylsilane
(prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 497180-99-1P 497181-00-7P 497181-01-8P 497181-02-9P
497181-03-0P 497181-04-1P 497181-05-2P
497181-06-3P 497181-07-4P
(protodesilylation; nucleophilic Michael addn. of silylated synthetic equiv. of benzyl mercaptans and thiophenols with subsequent protodesilylation)

IT 20591-87-1P
(redn. product; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their addn. and redn. reactions and desilylation)

IT 2531-80-8
(redn.; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their addn. and redn. reactions and desilylation)

IT 497180-96-8P 497180-97-9P 497180-98-0P
(redn.; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 95-46-5 106-38-7 591-17-3
(silylation; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 637-59-2
(thioetherification; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their substitution reactions and desilylation)

IT 17903-42-3 17903-43-4 17903-44-5
(thiolation; prepn. of low-**odor** silylated synthetic

equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 19061-64-4P 497180-86-6P 497180-87-7P 497180-88-8P 497180-89-9P 497180-90-2P
(thiolation; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 497181-11-0P
(thiophenol addn. product; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their addn. and redn. reactions and desilylation)

IT 2216-94-6, Ethyl phenylpropiolate
(thiophenol radical addn.; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their addn. and redn. reactions and desilylation)

IT 3644-91-5 18412-77-6 18412-78-7
(α-bromination; prepn. of low- **odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 3728-43-6P 3728-44-7P 7450-03-5P 17897-71-1P 497180-91-3P 497180-92-4P
(α-bromination; prepn. of low- **odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

L40 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

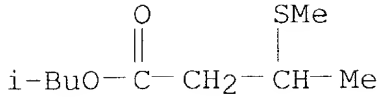
1990:439170 Document No. 113:39170 Alkyl (3-methylthio)-butyrates, their preparation and use as fruit **flavoring** agents. Bruijnje, Arnold; Heideman, Theo; Wille, Hans Julius (Naarden International N. V., Neth.). Eur. Pat. Appl. EP 330254 A1 19890830, 6 pp. DESIGNATED STATES: R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1989-200313 19890210. PRIORITY: NL 1988-502 19880226.

AB CH3CH(SH)CH2CO2R (R = C4-5 optionally branched alkyl) is manufd. and used as a **flavoring** agent imparting fresh fruit **flavor**. Thus, iso-Bu (3-methylthio)-butyrate (I) was prepd. from Na methoxide, isobutylcrotonate, and methylmercaptan with a yield of 88%. Prepn. of a strawberry **flavor compn** . contg. I and its use in manufg. strawberry jam were also disclosed.

IT **127931-21-9P**
(manuf. of, as fruit **flavoring** agent)

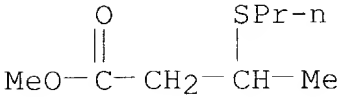
RN 127931-21-9 HCAPLUS

CN Butanoic acid, 3-(methylthio)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

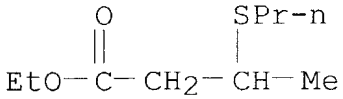


IC ICM C07C149-20
ICS A23L001-226
CC 17-6 (Food and Feed Chemistry)
ST butyrate fruit **flavor** agent manuf; strawberry **flavor** butyrate
IT **Flavoring** materials
(fruit, alkylmethylthiobutyrates, prepn. and use of)
IT **Flavoring** materials
(strawberry, isobutylmethylthio butyrate, prepn. and use of)
IT Jams and Jellies
(strawberry, strawberry-**flavored**, manuf. of, isobutylmethylthio butyrate prepn. in relation to)
IT Milk preparations
(yogurt, strawberry-**flavored**, manuf. of, isobutylmethylthio butyrate prepn. in relation to)
IT 74-93-1, Methylmercaptan, biological studies 124-41-4 589-66-2, Isobutylcrotonate
(in **flavoring** agent butyrate manuf.)
IT **127931-21-9P**
(manuf. of, as fruit **flavoring** agent)

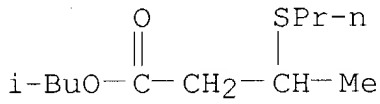
L40 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
1987:195056 Document No. 106:195056 Esters of alkylthioalkanoic acids as **aromas** and **flavors** for foods. Courtney, Thomas F., Jr.; Pittet, Alan O.; Muralidhara, Ranya; Vock, Manfred H.; Wiener, Charles (International Flavors and Fragrances Inc., USA). U.S. US 4631194 A 19861223, 49 pp. (English). CODEN: USXXAM. APPLICATION: US 1985-789162 19851206.
AB The **aroma** and **taste** of foods are enhanced by addn. of 0.001-250 ppm (by wt. of the food) of an ester of an alkylthioalkanoic acid. Thus, allyl-2(3-hydroxypropylthio)propionate, having a roasted, sesame **aroma** and **taste** profile at 2 ppm, was prepd. by reaction of 2-mercaptopropionic acid with allyl alc. in the presence of p-toluenesulfonic acid.
IT **108073-21-8P 108073-22-9P 108073-24-1P 108073-27-4P**
(prepn. of, as food **aroma** and **flavor** enhancer)
RN 108073-21-8 HCAPLUS
CN Butanoic acid, 3-(propylthio)-, methyl ester (9CI) (CA INDEX NAME)



RN 108073-22-9 HCAPLUS
CN Butanoic acid, 3-(propylthio)-, ethyl ester (9CI) (CA INDEX NAME)

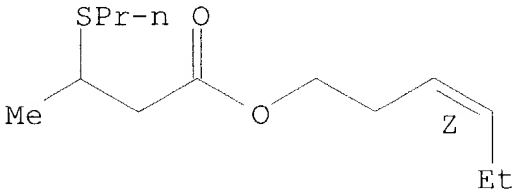


RN 108073-24-1 HCAPLUS
CN Butanoic acid, 3-(propylthio)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



RN 108073-27-4 HCAPLUS
CN Butanoic acid, 3-(propylthio)-, 3-hexenyl ester, (Z)- (9CI) (CA INDEX NAME)

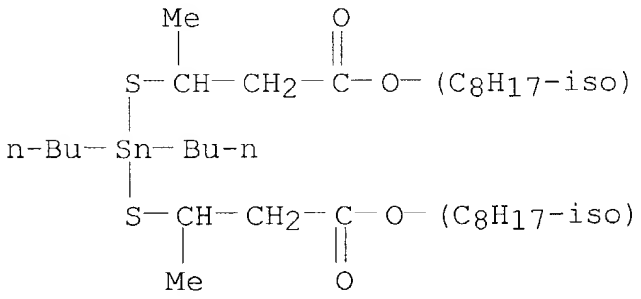
Double bond geometry as shown.



IC ICM A23L001-226
ICS A23L001-231; A23L001-235
NCL 426535000
CC 17-6 (Food and Feed Chemistry)
ST alkylthioalkanoic acid ester food **flavor aroma**; thioalkanoate alkyl ester food **flavor aroma**
IT **Flavoring** materials
(alkylthioalkanoic acid esters)
IT **Odor** and **Odorous** substances

(alkylthioalkanoic acid esters, for food)
IT Carboxylic acids, esters
(alkylthio, esters, as **aroma** and **flavor** substances for foods)
IT 90113-14-7P 108073-20-7P **108073-21-8P**
108073-22-9P 108073-23-0P **108073-24-1P**
108073-25-2P 108073-26-3P **108073-27-4P** 108073-28-5P
108073-29-6P
(prepn. of, as food **aroma** and **flavor** enhancer)

L40 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
1970:112263 Document No. 72:112263 Organotin stabilizers. Stapfer, Christian H. (Carlisle Chemical Works, Inc.). Fr. FR 1578260 19690814, 7 pp. (French). CODEN: FRXXAK. PRIORITY: US 19670719.
AB Dibutyltin azelate (I) or bis[(carbisooctoxymethylthio)dibutyltin] azelate and dibutyltin bis(isooctyl mercaptoacetate) (II) or dibutyltin bis(isooctyl 3-mercaptobutyrate) are used as efficient internal lubricants having no undesirable **odor** during extrusion of poly(vinyl chloride) (III). Thus, III contg. 0.5% I and 1.5% II had an extrusion index of 42 kg/hr as compared with 36.6 kg/hr for III contg. 2.5% II.
IT **26898-05-5**
(stabilizers, for vinyl chloride polymers, internal lubrication in relation to)
RN 26898-05-5 HCAPLUS
CN Butyric acid, 3,3'-[(dibutylstannylene)dithio]di-, diisooctyl ester (8CI) (CA INDEX NAME)



IC C07F; C08F
CC 36 (Plastics Manufacture and Processing)
IT 25168-24-5 **26898-05-5** 26898-06-6 27468-47-9
(stabilizers, for vinyl chloride polymers, internal lubrication in relation to)

L40 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

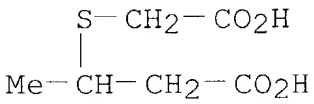
1957:40568 Document No. 51:40568 Original Reference No. 51:7607f-i
The **flavor** problem of soybean oil. XIII. Sulfur coordination compounds effective in edible-oil stabilization.
Schwab, A. W.; Moser, Helen A.; Gurley, Rosemary S.; Evans, C. D. (Northern Regional Research Lab., Peoria, IL). J. Am. Oil Chemists' Soc., 30, 413-17 (Unavailable) 1953.

AB cf. C.A. 47, 6569f. S compds. of the tridentate class having at least 2 COOH groups in α- or β-position to the coordinate atom are effective in stabilization of soybean oil. Among comparative model compds. with different coordinating atoms, the order of effectiveness appears to be S > N > O. (Carboxymethylthio)butyric acid, (carboxymethylthio)phenylpropionic acid, the monoethyl ester of (carboxymethylthio)succinic acid, p-toluenesulfonic acid, α,α'-thiodicaproic acid, and SO2 all improve the oxidative stability but gave undesirable **flavors**. Thiodiacetic acid, β,β'-thiodipropionic acid, (carboxymethylthio)succinic acid (I), and monooctadecyl ester of I were excellent stabilizers. The first 2 can be added either on the upgrade or the downgrade of deodorization, but the heat stability of the latter 2 limits their addn. to the downgrade. All these compds. improved the **flavor** stability as well as the oxidative stability. The monooctadecyl ester has the added advantage in that it is oil-sol.

IT **4386-05-4**, Butyric acid, 3-(carboxymethylthio)-
(soybean oil **flavor** and oxidative stabilization by)

RN 4386-05-4 HCAPLUS

CN Butanoic acid, 3-[(carboxymethyl)thio]- (9CI) (CA INDEX NAME)



CC 12 (Foods)

IT Soybean oil
(**flavor** and oxidative stabilization of, S coordination compds. in)

IT 99-68-3, Succinic acid, (carboxymethylthio)-
(and esters, soybean oil **flavor** and oxidative stabilization by)

IT 7704-34-9, Sulfur
(compds., soybean oil **flavor** and oxidative stabilization by)

IT 104-15-4, p-Toluenesulfonic acid 111-17-1, Propionic acid, 3,3'-thiodi- 123-93-3, Acetic acid, thiodi- 505-47-5, Propionic acid, 3,3'-iminodi- **4386-05-4**, Butyric acid, 3-(carboxymethylthio)- 5961-83-1, Propionic acid, 3,3'-oxydi-

67242-91-5, Hydrocinnamic acid, β-(carboxymethylthio)-
105910-65-4, Hexanoic acid, 2,2'-thiodi-
(soybean oil **flavor** and oxidative stabilization by)

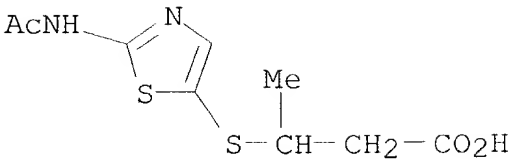
L40 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
1957:1799 Document No. 51:1799 Original Reference No. 51:395b-i,396a-d
The thiazole series. III. Sulfur-heterocyclic derivatives of 2-aminothiazole. Cagnoli, Nerina; Ricci, Adolfo (Univ. Perugia, Italy). Annali di Chimica (Rome, Italy), 46, 275-82 (Unavailable) 1956. CODEN: ANCRAI. ISSN: 0003-4592.
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 46, 496i; 50, 5564c. A number of derivs. have been prepd. from 2-amino-5-thiocyanothiazole, which has been prepd. from 2-aminothiazole and HSCN (C.A. 46, 496i). Thus, (2-acetamidothiazole-5-thio)propionic acid (I), white crystals, m. 185° (from alc.), was prepd. by adding 10 g. of (2-acetamido-5-thio)cyanothiazole (II) slowly to a freshly prepd. aq. soln. of 12 g. Na2S, heating to complete soln., cooling, decolorizing, and filtering off 2-acetamido-5-mercaptothiazole (III), which pptd. upon acidifying, redissolving 10 g. III in 2.3 g. NaOH in water, adding 9 g. BrCH2CH2CO2H, heating briefly until the color was light yellow, cooling, and pptg. by adding acid. I was also prepd. by adding 10 g. II to an aq. alc. soln. of 4 g. NaOH, heating to dissolve, adding an alk. soln. of 7.7 g. BrCH2CH2CO2H, heating until the reddish color lightened, cooling, and acidifying. Hydrolysis of I yielded (2-aminothiazole-5-thio)propionic acid, needles, m. 200-201° (from H2O). S.CHR.CH2.CO.C:C.S.C(NH2):N (IV) (R = H), straw-colored needles, m. 240-1°, formed when 2 g. of I was dissolved in 10 ml. concd. H2SO4, heated to 60-70° for 1 hr., poured into H2O pptg. the product, which was filtered off, and washed with H2O and Na2CO3 soln. The diazo deriv. of IV coupled with PhNMe2 yielded a dark red dye, m. 228-9° (from MeOH). Other derivs. were 2-acetyl-IV (R = H), white silky needles, m. 255-6° (from alc.), and IV-thiosemicarbazone (R = H), shiny whitish needles, m. 230-1° (from alc.), prepd. by dissolving 1 g. IV in a little alc., adding a few drops of 30% alc. HCl, heating, adding 0.5 g. thiosemicarbazide, heating, and collecting the ppt. for purification. β-Methyl(2-acetamidothiazole-5-thio)propionic acid (V), C9H12O3N2S2, white silky needles, m. 188-9° (from H2O), was made from II and β-bromobutyric acid as described above. IV (R = Me) (VI), yellow needles, m. 269-70° (decompn.) (from alc.) was likewise prepd. from V. 2-Acetyl-VI, needles, m. 288-9°, sol. in NaOH. VI thiosemicarbazone, m. 252-3° (from alc.). (2-Acetamidothiazole-5-thio)propanediol, white crystals, m. 165-6°, was prepd. by dissolving 10 g. III and 2.3 g. NaOH in hot alc. and adding 6.5 g. glycerol α-monochlorohydrin and heating 2 hrs., cooling, filtering off

the product and crystg. it from alc. The product was hydrolyzed to (2-aminothiazole-5-thio)propanediol, white needles, m. 115-16° (from H2O). S.C(NHAc):N.CH:CSC6H3(CO2H)NO2-2,4 (VII), obtained as its Na salt, golden-yellow scales, m. 322-3°, was prepd. from 10 g. III, and 2.3 g. NaOH in alc., 5 g. NaHCO3, and 11.6 g. 2-chloro-5-nitrobenzoic acid in alc. by refluxing 2 hrs., cooling, collecting the pptd. Na salt, and crystg. from hot H2O. The 2-H2N analog, yellow crystals, m. 257-8° (from alc., decompn.), was prepd. by acid hydrolysis of VII. VIIa, orange-yellow needles, m. 340°, was prepd. by treating VII with 10 ml. concd. H2SO4 and 2 g. P2O5 for 1 hr. at 70-80°, leaving overnight, pouring into ice, collecting the ppt., washing with Na2CO3, drying at 80°, and crystg. from PhNO2. 4-Oxo-2-acetamido-4,5-dihydrothieno[2,3-b]thiazole, white crystals, m. above 320°, was prepd. (1 g. yield) by suspending 10 g. S-(2-acetamido-5-thiazolyl)thioglycolic acid in 50 ml. POCl3 and refluxing 2-3 hrs., distilling off the excess POCl3, pouring into ice water, neutralizing with Na2CO3, and collecting the brick-red ppt. from AcOH. 2-Acetamido-5-thiazolyl 2-nitrophenyl sulfide (VIII), white needles, m. 225-6° (from alc.), was prepd. by adding 10 g. III to an alc. soln. of 2.3 g. NaOH, taking to a boil, adding 7.2 g. 2-ClC6H4NO2 in alc., refluxing 4 hrs., cooling, distg. off most of the alc., collecting the ppt., and crystg. from alc. 2-Acetamido-5-thiazolyl 2-aminophenyl sulfide, bunches of white needles, m. 217-18° (from alc.), was prepd. by suspending 10 g. VIII in a little alc., adding 50 ml. NH4OH and 20 ml. H2O, heating to 60-70°, adding a soln. of 66 g. FeSO4 in water, agitating 1 hr., filtering the cooled soln., extg. the ppt. with hot alc., and purifying by extg. with dil. HCl and repptg. Diazotized and decompd., this yielded a product, m. 120-4°, with an **odor** resembling that of PhNO2 (cf. Cullinane, et al., C.A. 31, 3987). 2-Acetamido-5-thiazolyl 2,4-dinitrophenyl sulfide, yellow needles, m. 294-5° (from alc.), was prepd. from 10 g. III, 2.3 g. NaOH, and 11.6 g. 2,4-(O2N)2C6H3Cl in the described manner. VIIIa, small shiny crystals, m. 247-8°, was prepd. by dissolving 5 g. 3-methyl-5-aminothianaphthene in a little AcOH, cooling to 0°, and adding slowly 1.75 ml. Br2 in AcOH. Thiocyanation yielded a white cryst. material which is poured into H2O, neutralized with Na2CO3, and crystd. from alc.

IT **99362-84-2**, Butyric acid, 3-(2-acetamido-5-thiazolylthio)- (prepn. of)

RN 99362-84-2 HCAPLUS

CN Butyric acid, 3-(2-acetamido-5-thiazolylthio)- (6CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT 98134-99-7, Propionic acid, 3-(2-amino-5-thiazolylthio)-
98489-98-6, 1,2-Propanediol, 3-(2-acetamido-5-thiazolylthio)-
99073-61-7, Benzoic acid, 2-(2-amino-5-thiazolylthio)-5-nitro-
99362-84-2, Butyric acid, 3-(2-acetamido-5-thiazolylthio)-
99848-24-5, 1,2-Propanediol, 3-(2-amino-5-thiazolylthio)-
99973-26-9, Thiazole, 2-acetamido-5-(o-nitrophenylthio)-
99974-43-3, Thiazole, 2-acetamido-5-(2,4-dinitrophenylthio)-
100377-69-3, Propionic acid, 3-(2-acetamido-5-thiazolylthio)-
108249-46-3, 7H-Thiopyrano[3,2-d]thiazol-7-one, 2-amino-5,6-dihydro-6-methyl-, thiosemicarbazone 108480-68-8, 7H-Thiopyrano[3,2-d]thiazol-7-one, 2-acetamido-5,6-dihydro- 108845-52-9, 9H-[1]Benzothiopyrano[3,2-d]thiazol-9-one, 2-acetamido-7-nitro-
110937-01-4, Thiazole, 2-acetamido-5-(o-aminophenylthio)-
114794-02-4, 7H-Thiopyrano[3,2-d]thiazol-7-one, 2-amino-5,6-dihydro-6-methyl- 115247-56-8, Thieno[3,2-f]benzothiazole, 2-amino-7-methyl- 117883-91-7, Benzoic acid, 2-(2-acetamido-5-thiazolylthio)-5-nitro-, sodium salt 119248-31-6, 7H-Thiopyrano[3,2-d]thiazol-7-one, 2-amino-5,6-dihydro-, thiosemicarbazone 120208-30-2, Thieno[3,2-d]thiazol-6(5H)-one, 2-acetamido- 120267-20-1, 7H-Thiopyrano[3,2-d]thiazol-7-one, 2-amino-5,6-dihydro- 120944-93-6, 7H-Thiopyrano[3,2-d]thiazol-7-one, 2-acetamido-5,6-dihydro-5-methyl-
(prepn. of)